WETTABILITY AND ADHESION WORK PREDICTION IN THE POLYMER-AQUEOUS SOLUTION OF SURFACE ACTIVE AGENT SYSTEMS

ANNA ZDZIENNICKA[1], JOANNA KRAWCZYK[1] AND BRONISŁAW JAŃCZUK[1,*]

[1]Department of Interfacial Phenomena, Faculty of Chemistry, Maria Curie-Skłodowska University, Maria Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland
aniaz@hektor.umcs.lublin.pl (A.Z.); j.krawczyk@poczta.umcs.lublin.pl (J.K.)

*Correspondence: bronislaw.janczuk@poczta.umcs.lublin.pl; Tel.: (48-81) 537-56-70

Running title: Wettability and adhesion work prediction

Fig. S1

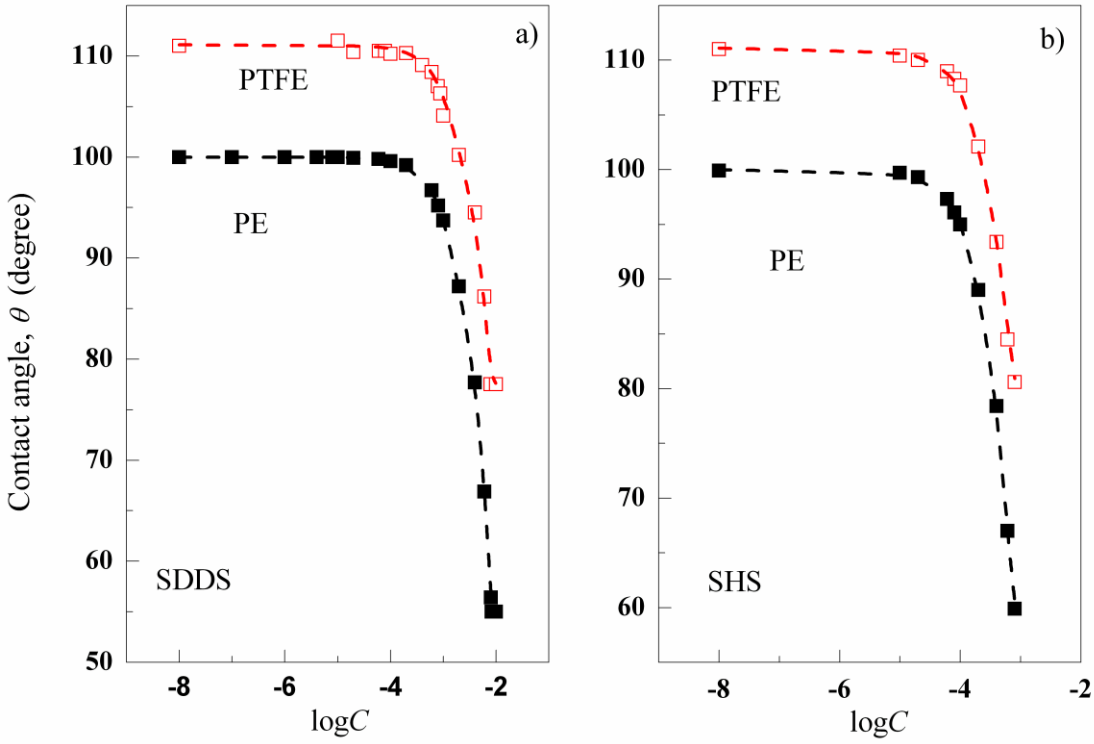

Fig. S1. A plot of the contact angle of the aqueous solution of SDDS (a) and SHS (b) (θ) on PE and PTFE surface vs. logarithm of surfactant concentration (C). Points correspond to the measured θ values on PTFE (from ref [18]) and on PE. Dash lines correspond to θ calculated form Eq. (15).

Fig. S2

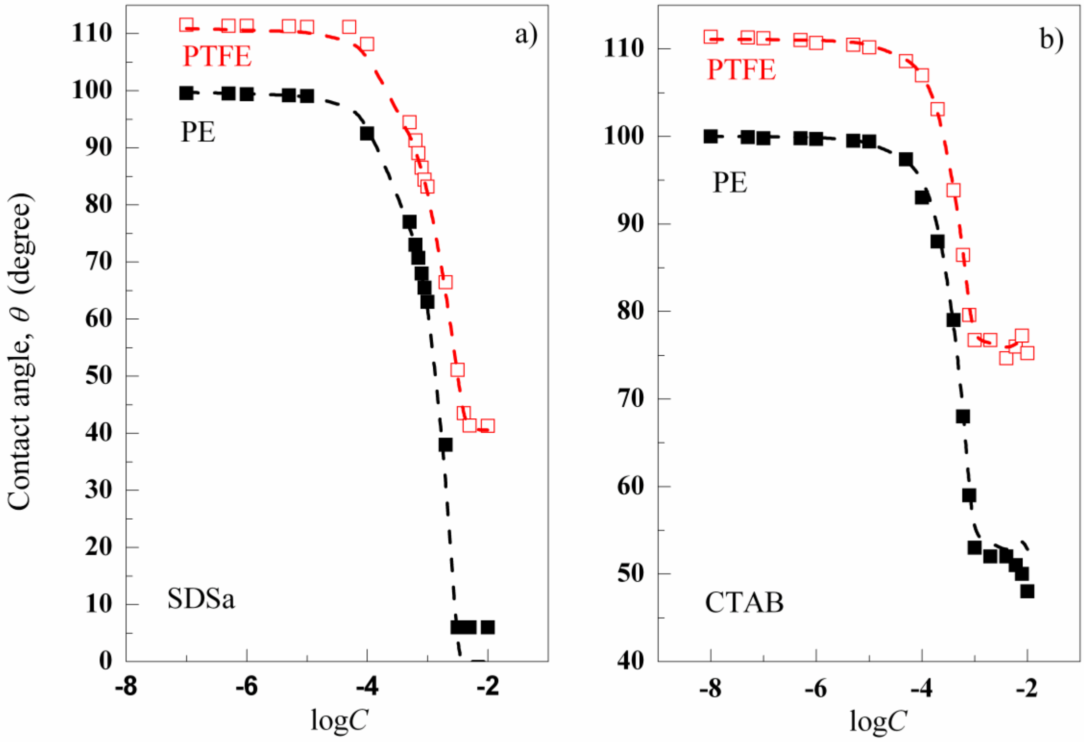

Fig. S2. A plot of the contact angle of the aqueous solution of SDSa (a) and CTAB (b) (θ) on PE and PTFE surface vs. logarithm of surfactant concentration (C). Points correspond to the measured θ values on PTFE (from ref [18]) and on PE. Dash lines correspond to θ calculated form Eq. (15).

Fig. S3

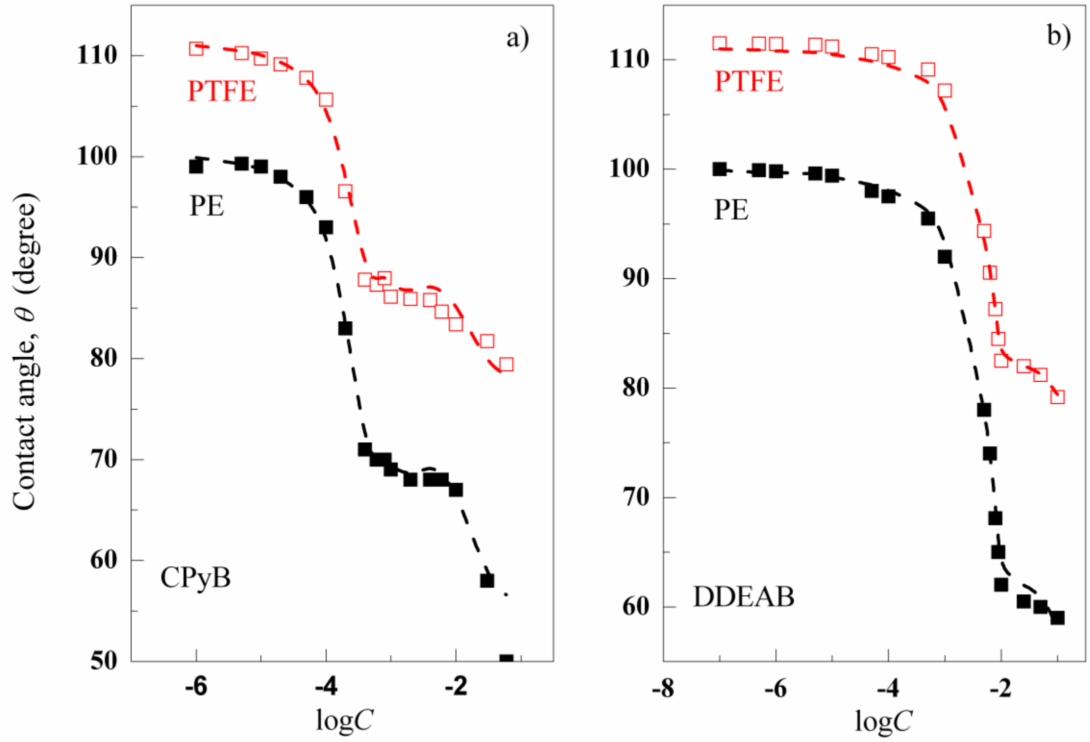

Fig. S3. A plot of the contact angle of the aqueous solution of CPyB (a) and DDEAB (b) (θ) on PE and PTFE surface vs. logarithm of surfactant concentration (C). Points correspond to the measured θ values on PTFE (from ref [18]) and on PE. Dash lines correspond to θ calculated form Eq. (15).

Fig. S4

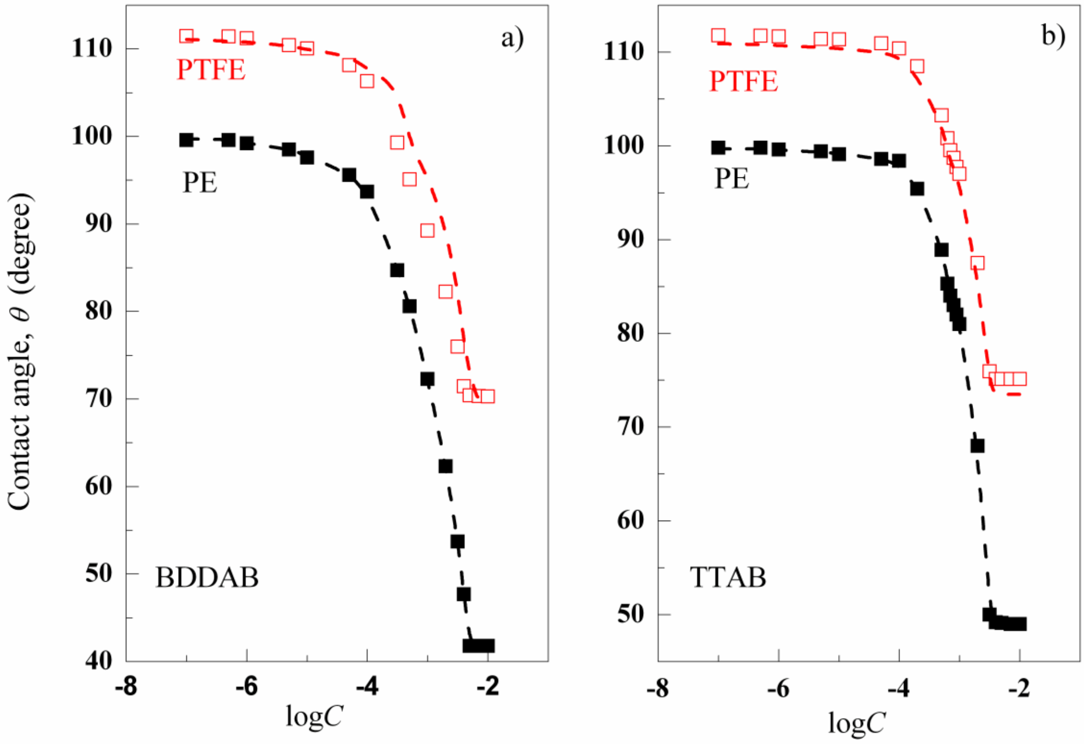

Fig. S4. A plot of the contact angle of the aqueous solution of BDDAB (a) and TTAB (b) (θ) on PE and PTFE surface vs. logarithm of surfactant concentration (C). Points correspond to the measured θ values on PTFE (from ref [18]) and on PE. Dash lines correspond to θ calculated form Eq. (15).

Fig. S5

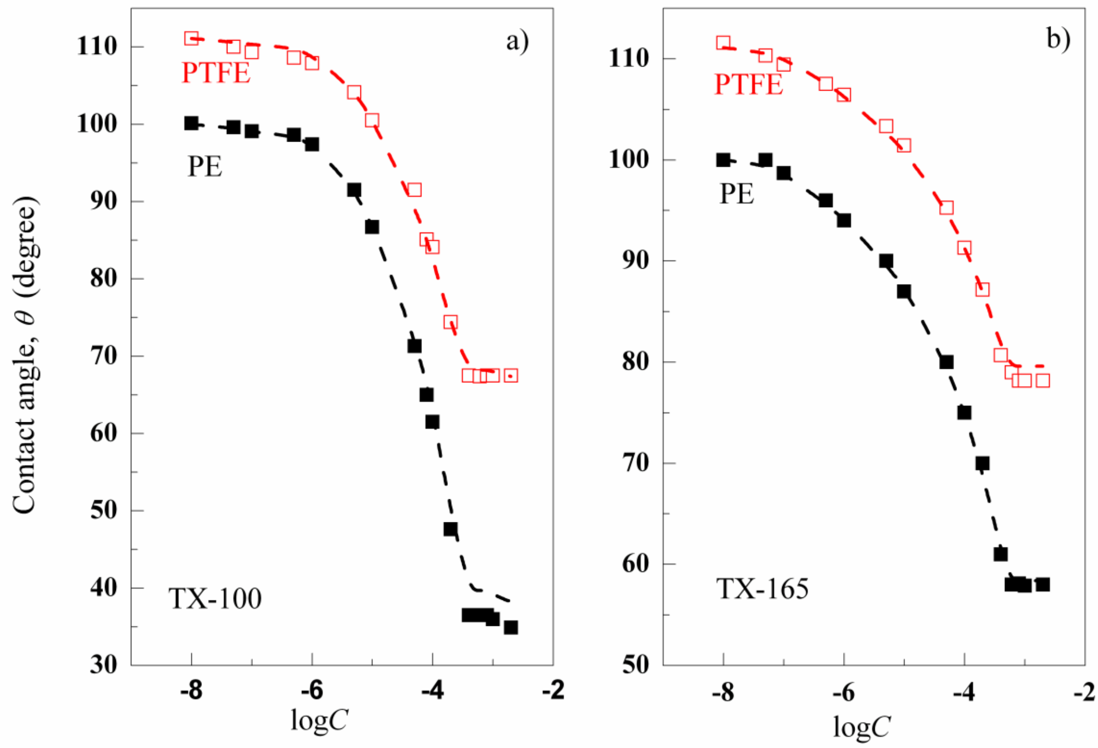

Fig. S5. A plot of the contact angle of the aqueous solution of TX-100 (a) and TX-165 (b) (θ) on PE and PTFE surface vs. logarithm of surfactant concentration (C). Points correspond to the measured θ values on PTFE (from ref [18]) and on PE. Dash lines correspond to θ calculated form Eq. (15).

Fig. S6

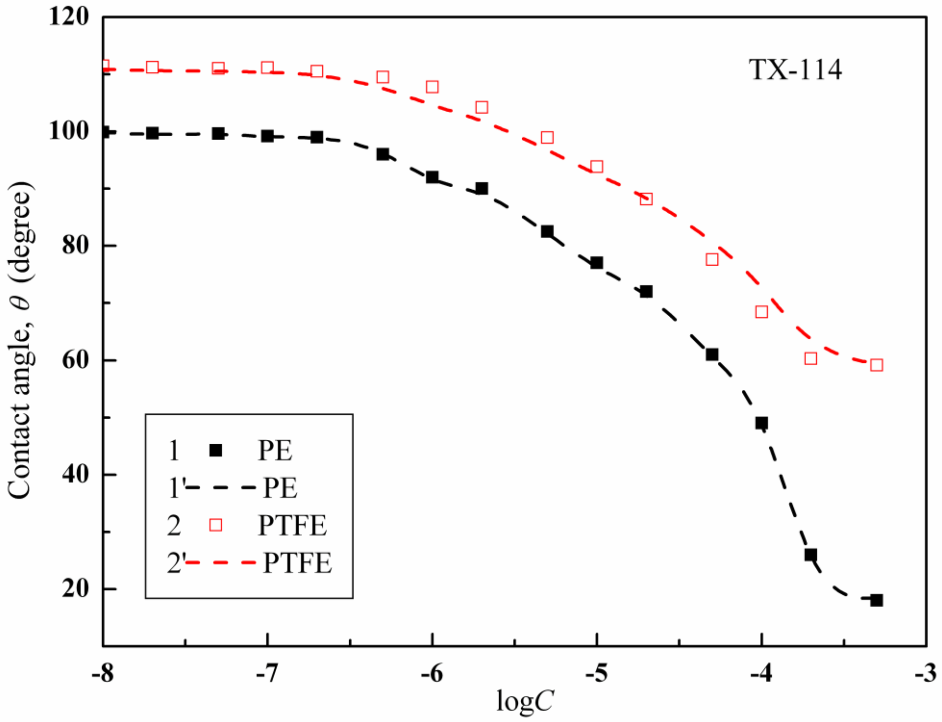

Fig. S6. A plot of the contact angle of the aqueous solution of TX-114 (θ) on PE and PTFE surface vs. logarithm of surfactant concentration (C). Points correspond to the measured θ values on PTFE (from ref [18]) and on PE. Dash lines correspond to θ calculated form Eq. (15).

Fig. S7

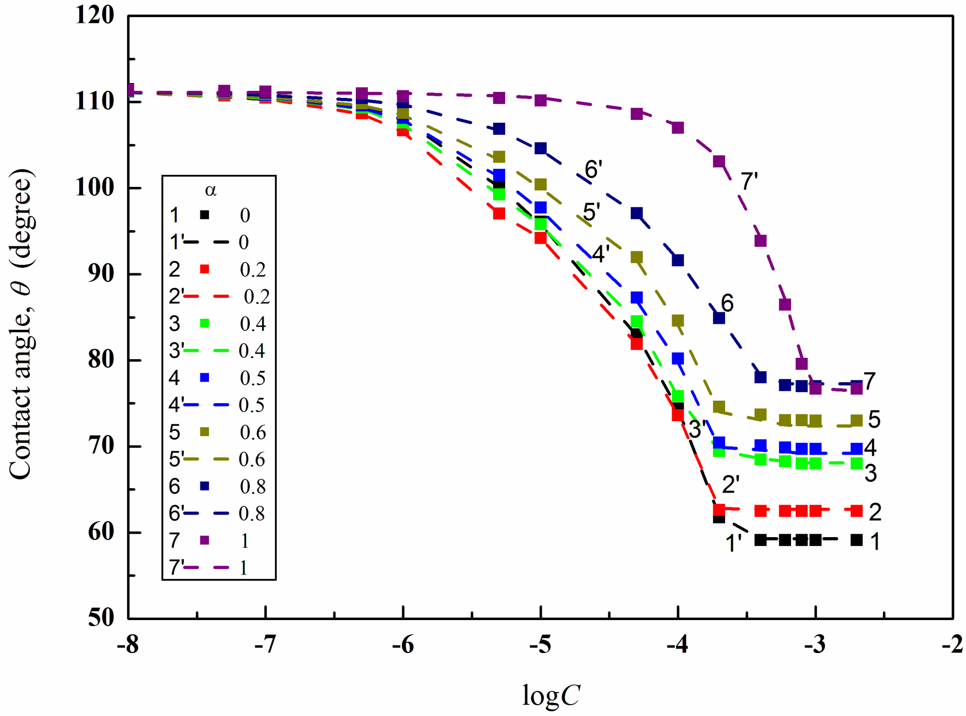

Fig. S7. A plot of the contact angle (θ) of the aqueous solutions of the TX-114+CTAB mixture on the PTFEE surface vs. the logarithm of the total concentration of the mixture (C). Points 1-7 correspond to θ values of the mixture with the mole fraction of CTAB in the bulk phase (α) equal to 0, 0.2, 0.4, 0.5, 0.6, 0.8 and 1, respectively, taken from ref. [16]. Dash lines $1'$-$7'$ correspond to θ values calculated from Eq. (15).

Fig. S8

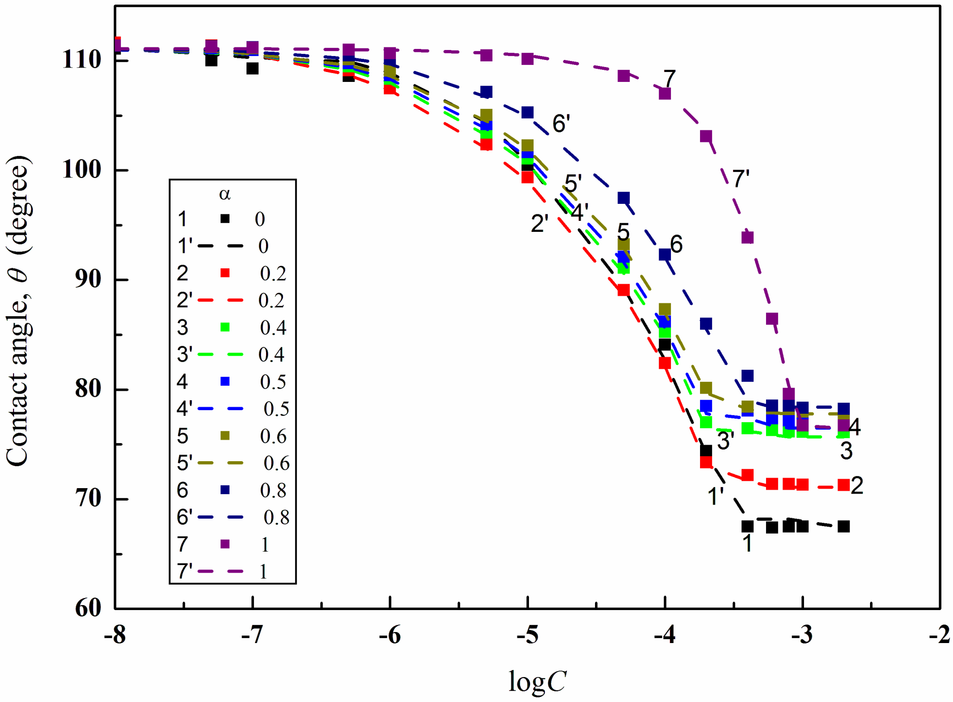

Fig. S8. A plot of the contact angle (θ) of the aqueous solutions of the TX-100+CTAB mixture on the PTFE surface vs. the logarithm of the total concentration of the mixture (C). Points 1-7 correspond to θ values of the mixture with the mole fraction of CTAB in the bulk phase (α) equal to 0, 0.2, 0.4, 0.5, 0.6, 0.8 and 1, respectively, taken from ref. [16]. Dash lines $1'$-$7'$ correspond to θ values calculated from Eq. (15).

Fig. S9

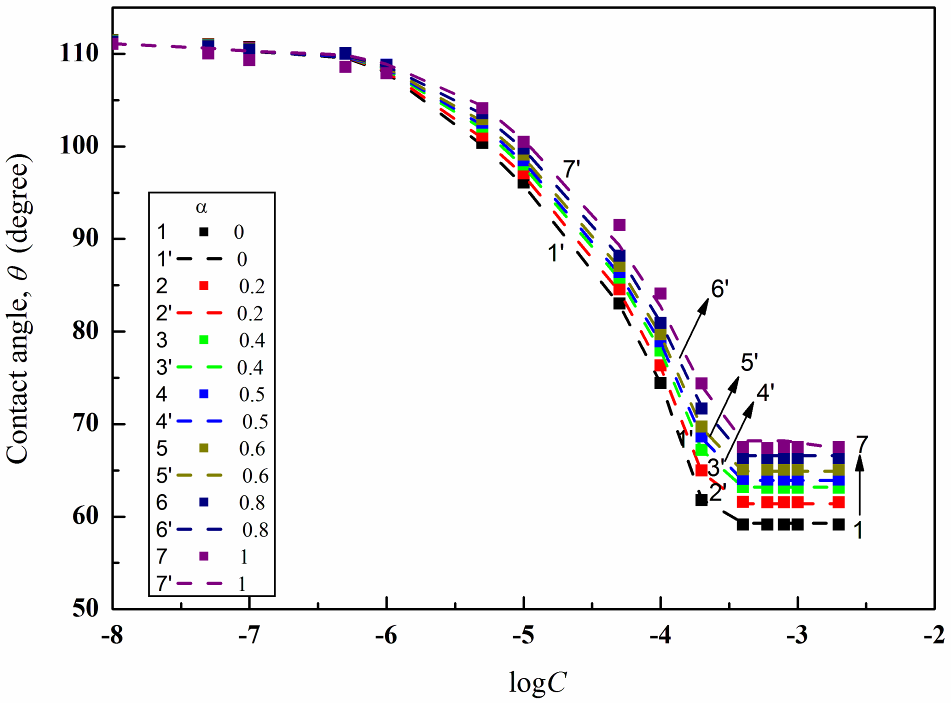

Fig. S9. A plot of the contact angle (θ) of the aqueous solutions of the TX-100+TX-114 mixture on the PTFE surface vs. the logarithm of the total concentration of the mixture (C). Points 1-7 correspond to θ values of the mixture with the mole fraction of TX-114 in the bulk phase (α) equal to 0, 0.2, 0.4, 0.5, 0.6, 0.8 and 1, respectively, taken from ref. [16]. Dash lines $1^{'}$-$7^{'}$ correspond to θ values calculated from Eq. (15).

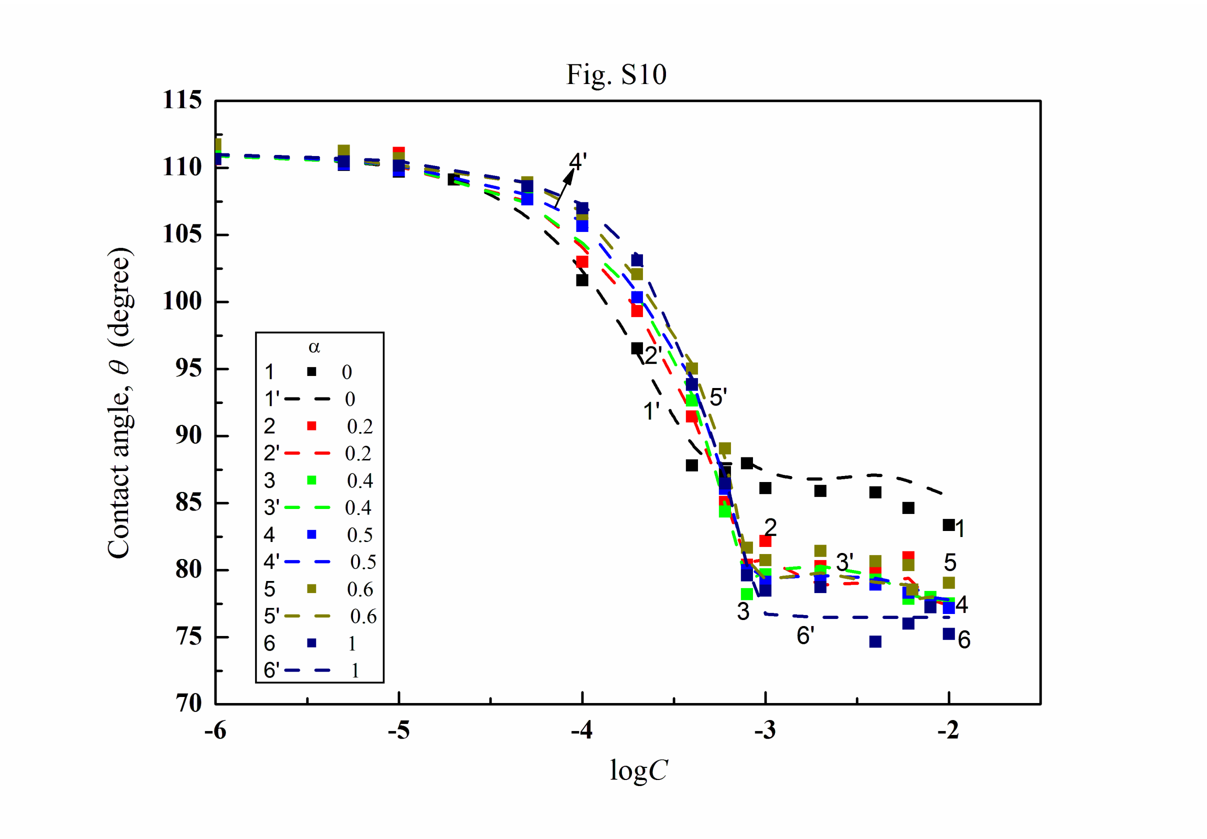

Fig. S10. A plot of the contact angle (θ) of the aqueous solutions of the CPyB+CTAB mixture on the PTFE surface vs. the logarithm of the total concentration of the mixture. Points 1-6 correspond to θ values of the mixture with the mole fraction of CTAB in the bulk phase (α) equal to 0, 0.2, 0.4, 0.6, 0.8 and 1, respectively, taken from ref. [14]. Dash lines $1^{'}$-$6^{'}$ correspond to θ values calculated from Eq. (15).

Fig. S11

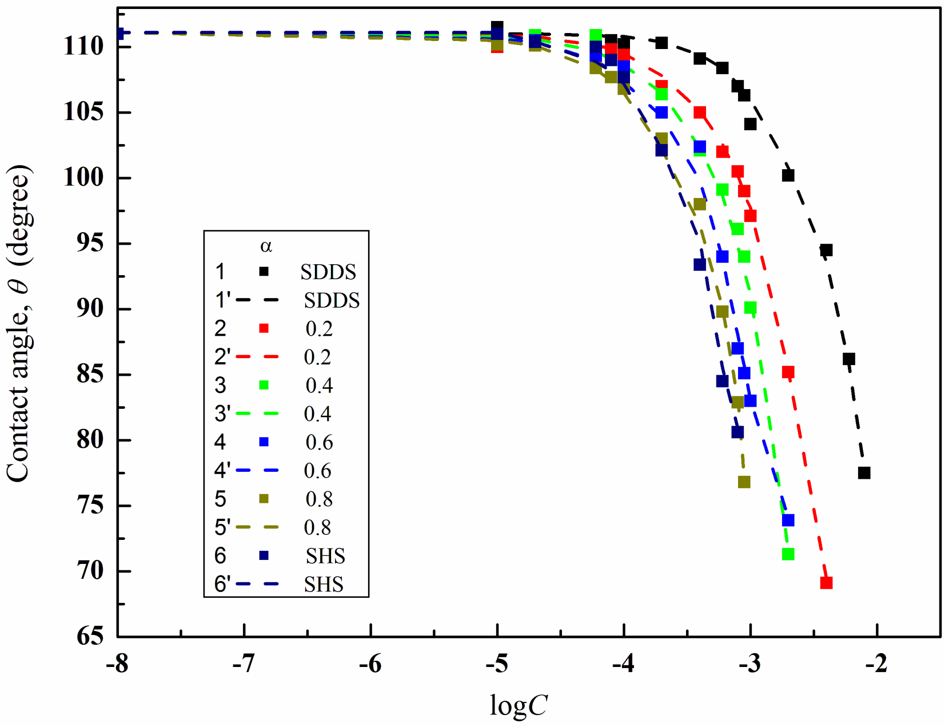

Fig. S11. A plot of the contact angle (θ) of the aqueous solutions of the SDDS+SHS mixture on the PTFE surface vs. the logarithm of the total concentration of the mixture. Points 1-6 correspond to θ values of the mixture with the mole fraction of SHS in the bulk phase (α) equal to 0, 0.2, 0.4, 0.6, 0.8 and 1, respectively, taken from ref. [14]. Dash lines $1^{'}$-$6^{'}$ correspond to θ values calculated from Eq. (15).

Fig. S12

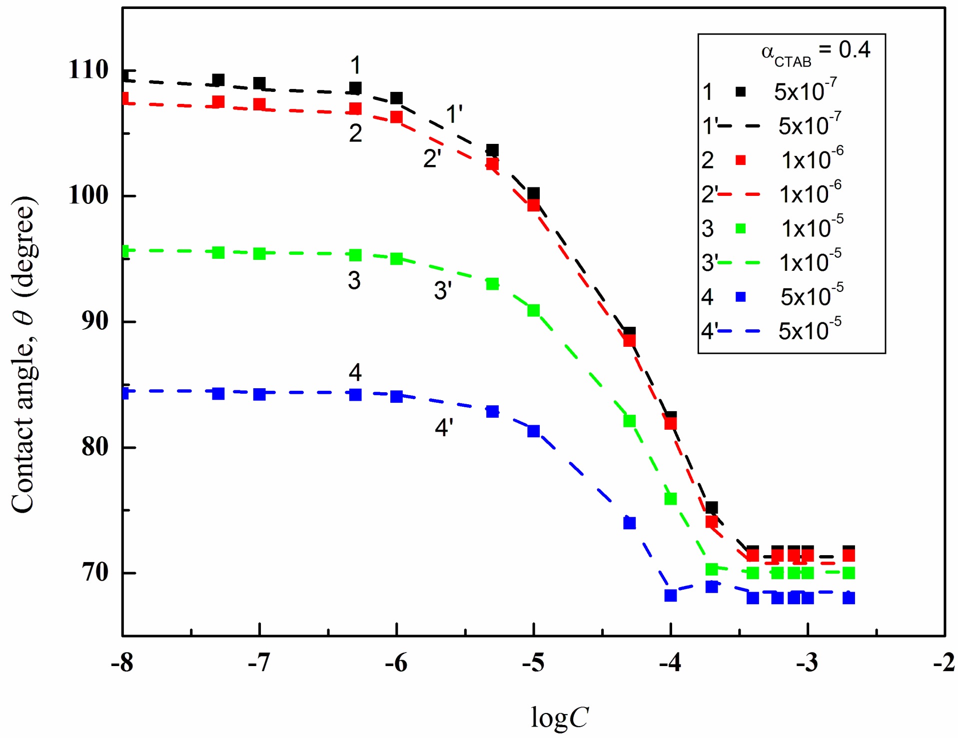

Fig. S12. A plot of the contact angle of the aqueous solution of TX-100+TX-114+CTAB mixture (θ) on PTFE surface vs. logarithm of the TX-100 concentration (C). For binary mixture at concentration equal to $5x10^{-7}$ M, $1x10^{-6}$ M, $1x10^{-5}$ M and $5x10^{-5}$ M the mole fraction of CTAB was constant and equal to 0.4. Points 1- 4 correspond to θ values from ref. [17]. Dash lines $1^{'}$-$4^{'}$ correspond to θ values calculated from Eq. (15).

Fig. S13

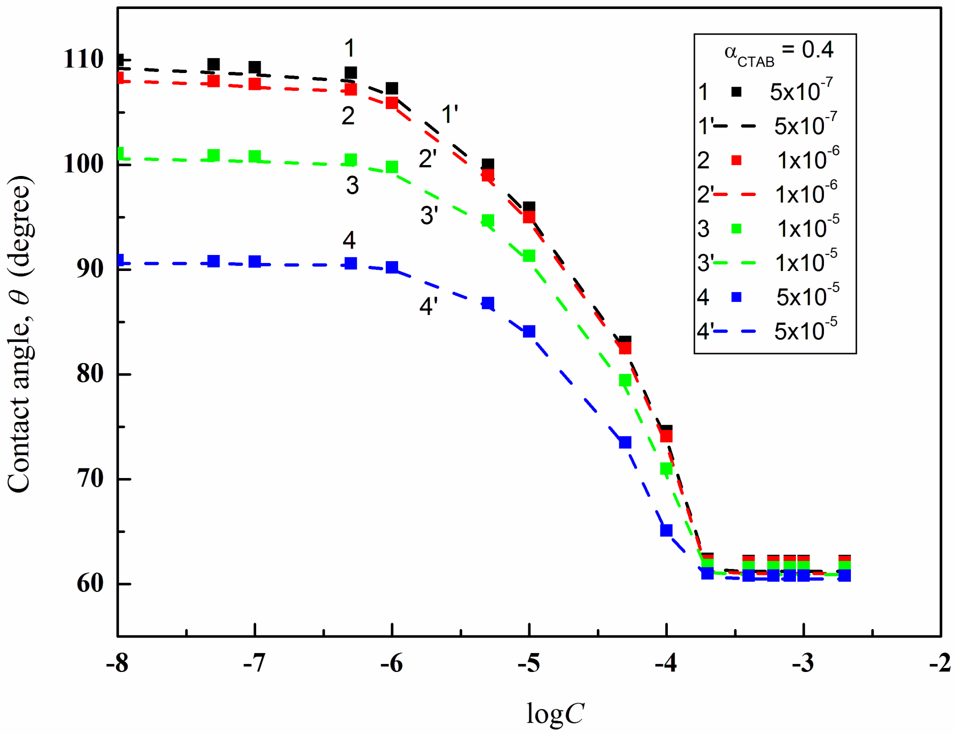

Fig. S13. A plot of the contact angle of the aqueous solution of TX-114+TX-100+CTAB mixture (θ) on PTFE surface vs. logarithm of the TX-114 concentration (C). For binary mixture at concentration equal to $5x10^{-7}$ M, $1x10^{-6}$ M, $1x10^{-5}$ M and $5x10^{-5}$ M the mole fraction of CTAB was constant and equal to 0.4. Points 1- 4 correspond to θ values from ref. [17]. Dash lines $1^{'}$-$4^{'}$ correspond to θ values calculated from Eq. (15).

Fig. S14

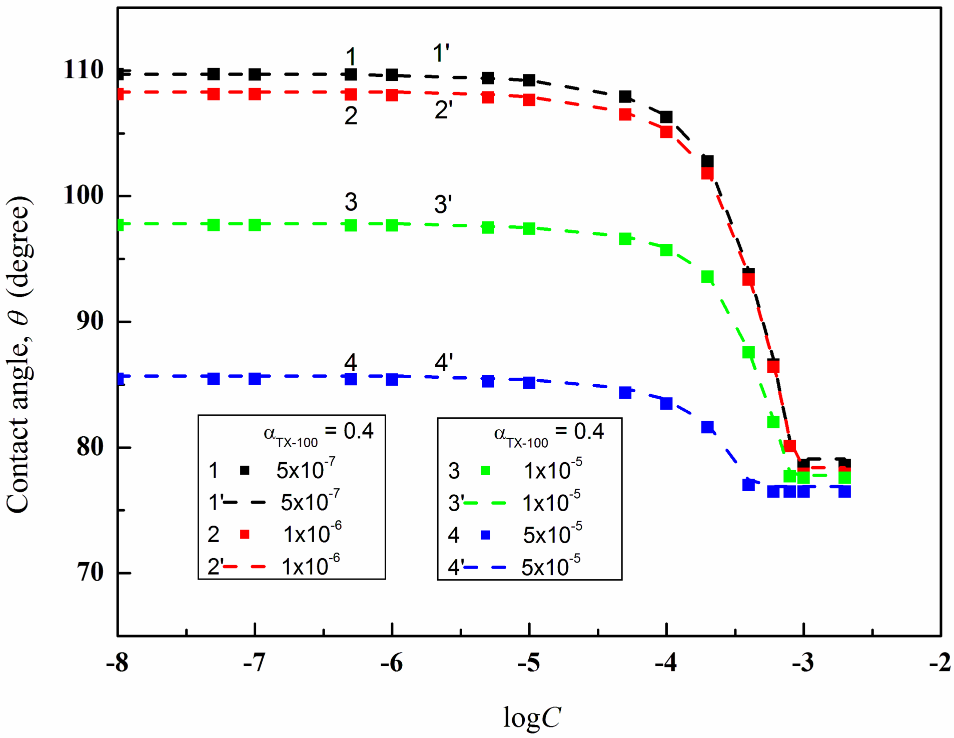

Fig. S14. A plot of the contact angle of the aqueous solution of CTAB+TX-114+TX-100 mixture (θ) on PTFE surface vs. logarithm of the CTAB concentration (*C*). For binary mixture at concentration equal to $5x10^{-7}$ M, $1x10^{-6}$ M, $1x10^{-5}$ M and $5x10^{-5}$ M the mole fraction of TX-100 was constant and equal to 0.4. Points 1- 4 correspond to θ values from ref. [17]. Dash lines $1^{'}$-$4^{'}$ correspond to θ values calculated from Eq. (15).

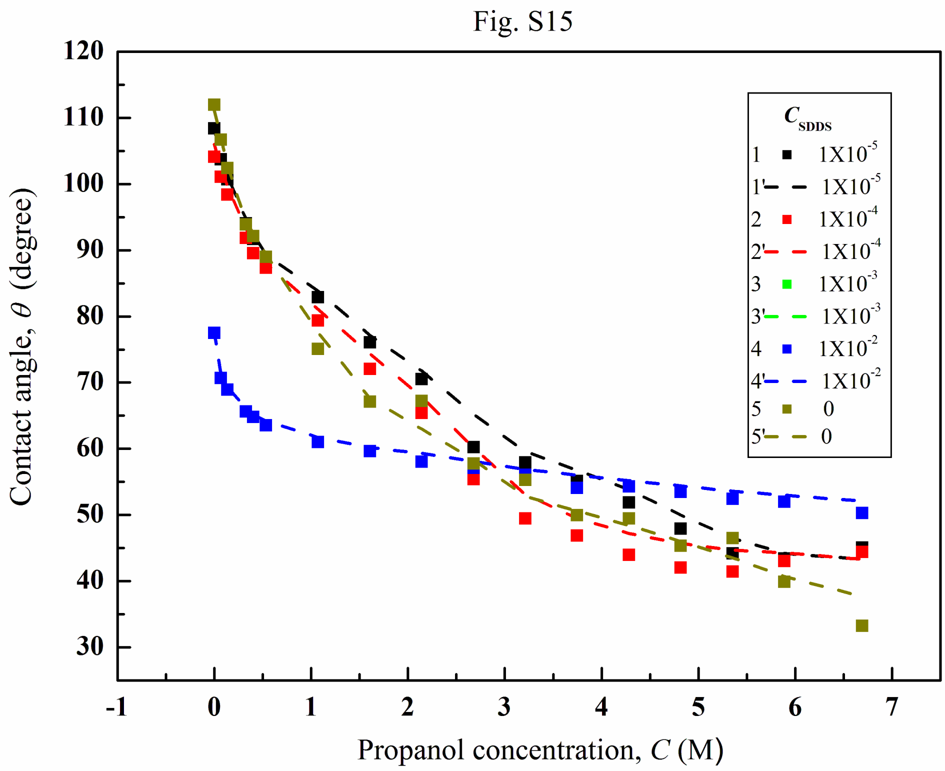

Fig. S15. A plot of the contact angle (θ) of the aqueous solutions of the SDDS in the presence of propanol on the PTFE surface vs. the concentration of propanol (C). Points 1-5 correspond to measured θ values of the SDDS mixture with propanol on PTFE surface at constant concentration of SDDS equal to $1x10^{-5}$ M, $1x10^{-4}$ M, $1x10^{-3}$ M, $5x10^{-2}$ M and 0 M, respectively, taken from ref. [11]. Dash lines $1'$-$5'$ correspond to θ values calculated from Eq. (15).

Fig. S16

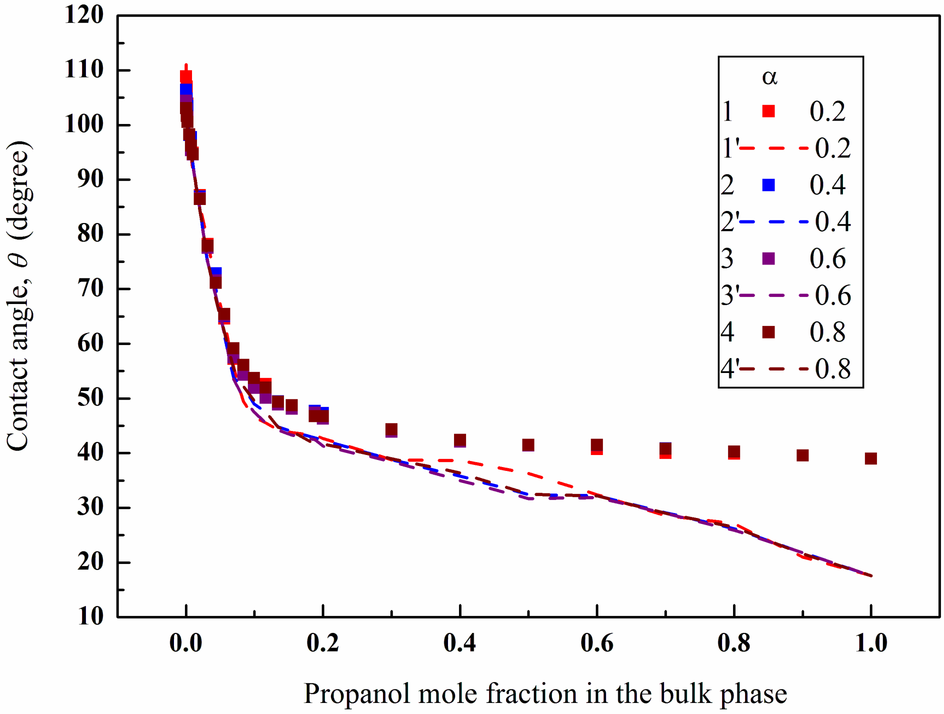

Fig. S16. A plot of the contact angle (θ) of the aqueous solutions of the SDDS+TX-100 in the presence of propanol on the PTFE surface as a function of propanol mole fraction in the bulk phase. Points 1-4 correspond to the measured θ values of the mixture with the mole fraction of TX-100 in the bulk phase (α) equal to 0.2, 0.4, 0.6 and 0.8, respectively at constant SDDS+TX-100 mixture concentration equal to $1x10^{-5}$ M, taken from ref. [37]. Dash lines $1'$-$4'$ correspond to θ values calculated from Eq. (15).

Fig. S17

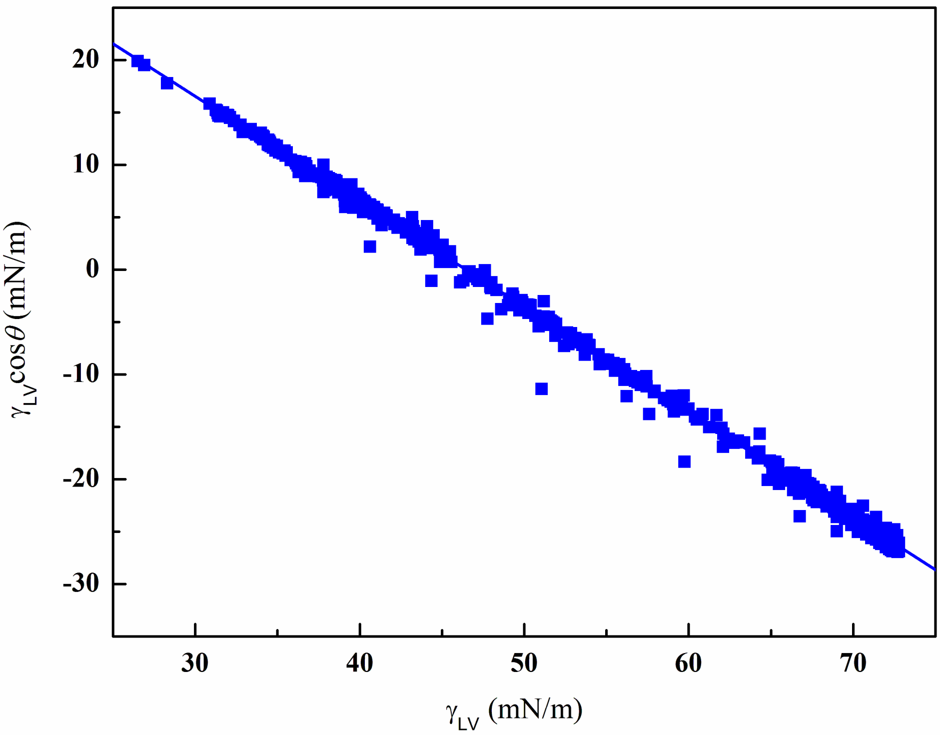

Fig. S17. The dependence between the adhesion ($\gamma_{LV}\cos\theta$) and surface tension (γ_{LV}) of the aqueous solutions of surfactants and their binary and ternary mixtures for the PTFE surface, from ref. [16-18].

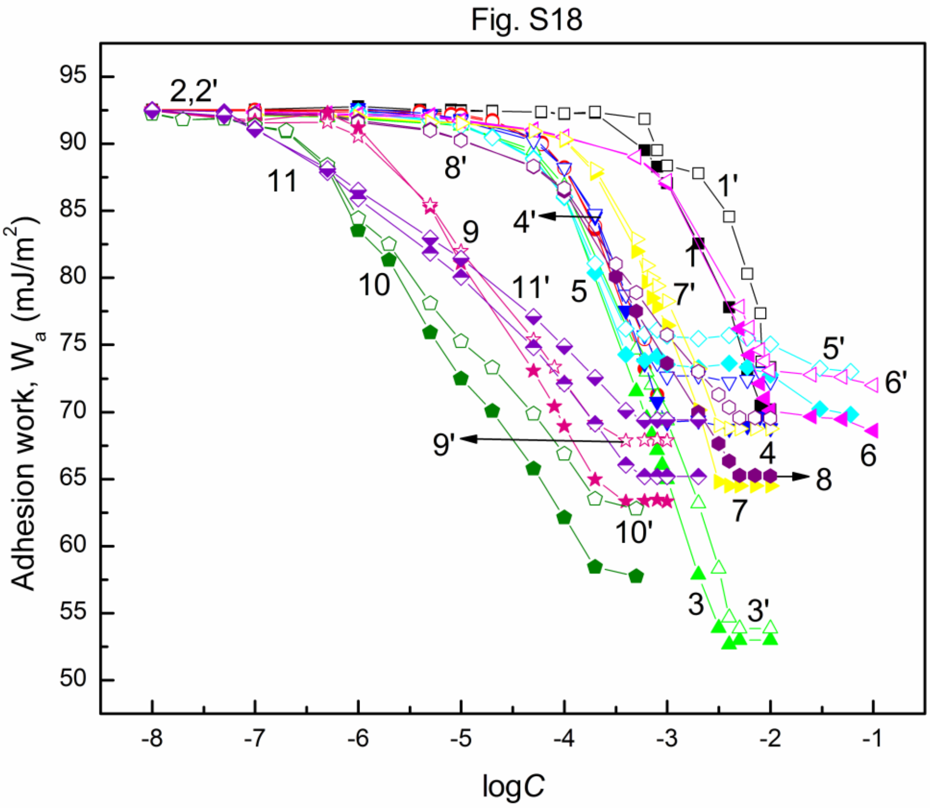

Fig. S18. A plot of the work of adhesion (W_a) of aqueous solutions of surfactants to the PMMA surface calculated from the Eq. (4) (curves 1 – 11) and Eq. (18) (curves 1' – 11') vs. the logarithm of surfactant concentration ($\log C$). Curves 1, 1'; 2,2'; 3,3'; 4, 4'; 5, 5'; 6, 6'; 7, 7', 8, 8'; 9, 9'; 10, 10' and 11, 11' correspond to the aqueous solution of SDDS, SHS, SDSa, CTAB, CPyB, DDEAB, TTAB, BDDAB, TX-100, TX-114 and TX-165, respectively.

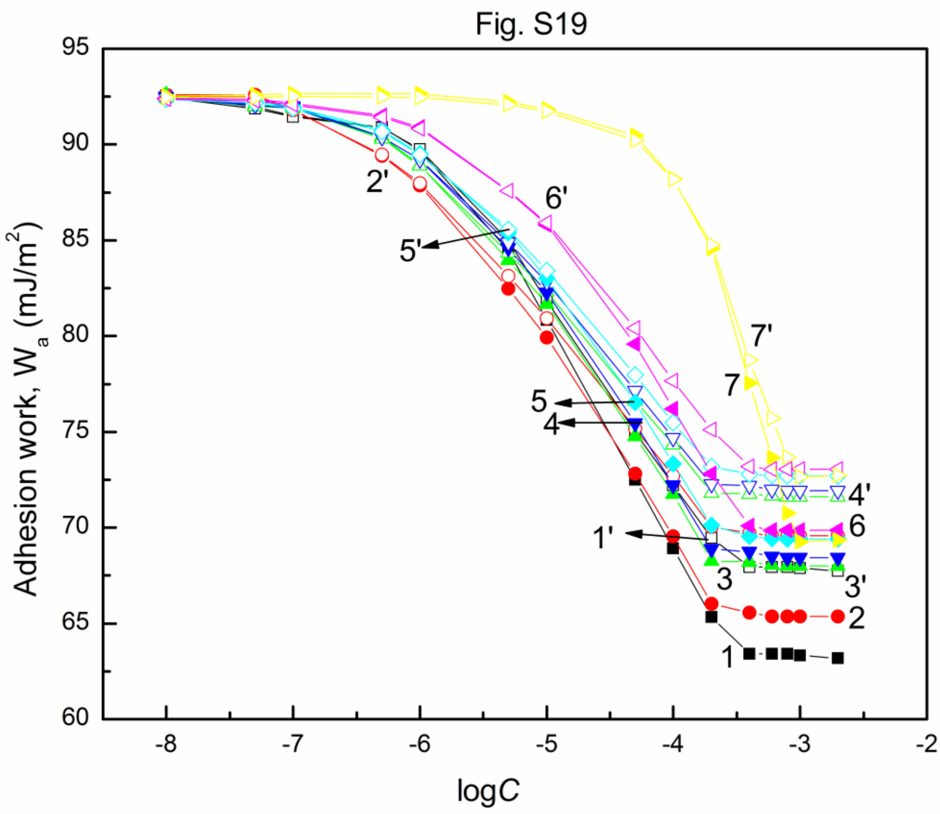

Fig. S19. A plot of the work of adhesion (W_a) of the aqueous solutions of CTAB and TX-100 mixtures to the PMMA surface calculated from the Eq. (4) (curves 1 – 7) and Eq. (18) (curves 1’ – 7’) vs. the logarithm of surfactant mixtures concentration ($\log C$). Curves 1, 1’; 2,2’; 3,3’; 4, 4’; 5, 5’; 6, 6’ and 7, 7’correspond to the CTAB mole fractions in the mixture equal to 0, 0.2; 0.4, 0,5; 0.6, 0.8 and 1, respectively.

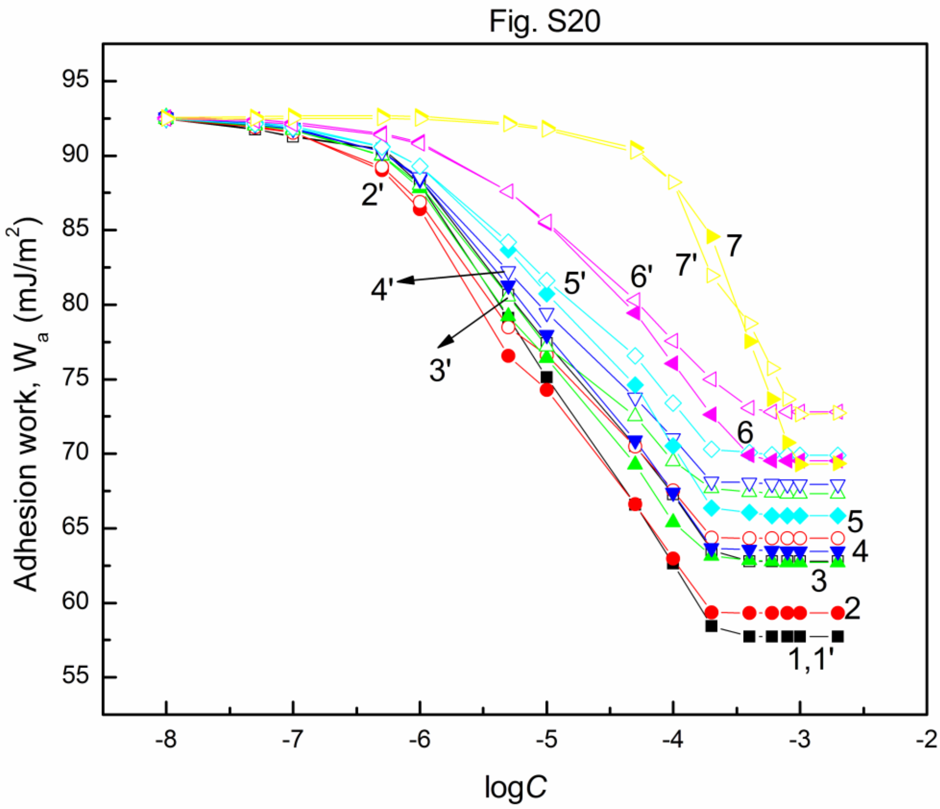

Fig. S20. A plot of the work of adhesion (W_a) of the aqueous solutions of CTAB and TX-114 mixtures to the PMMA surface calculated from the Eq. (4) (curves 1 – 7) and Eq. (18) (curves 1' – 7') vs. the logarithm of surfactant mixtures concentration ($\log C$). Curves 1, 1'; 2,2'; 3,3'; 4, 4'; 5, 5'; 6, 6' and 7, 7'correspond to the CTAB mole fractions in the mixture equal to 0, 0.2; 0.4, 0,5; 0.6, 0.8 and 1, respectively.

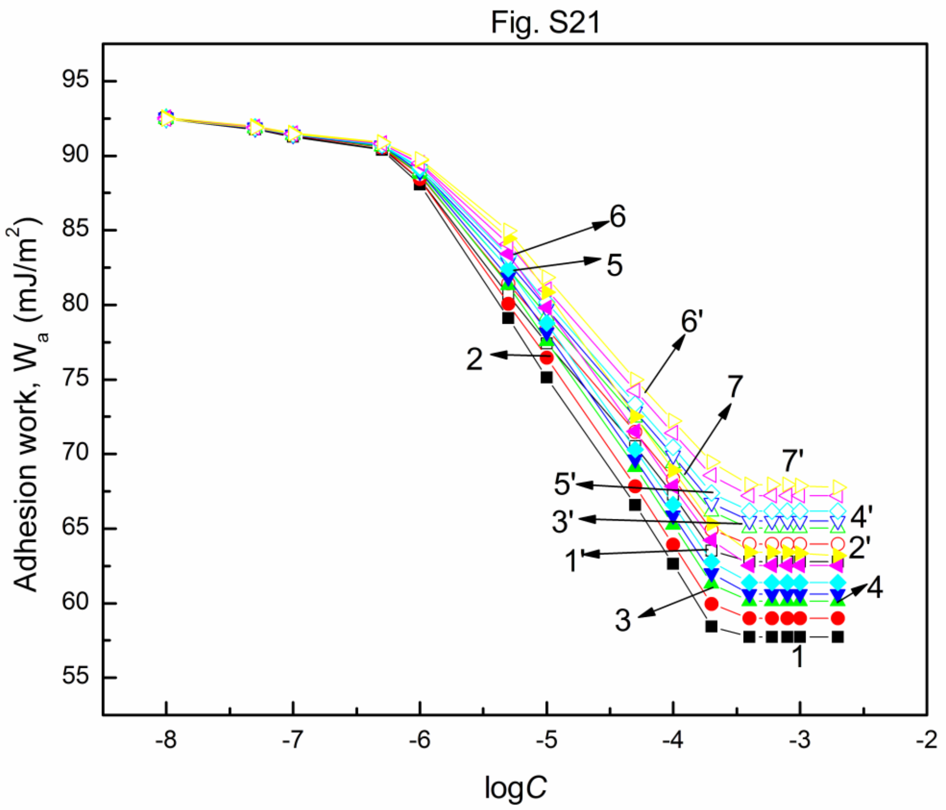

Fig. S21. A plot of the work of adhesion (W_a) of the aqueous solutions of TX-114 and TX-100 mixtures to the PMMA surface calculated from the Eq. (4) (curves 1 – 7) and Eq. (18) (curves 1' – 7') vs. the logarithm of surfactant mixtures concentration ($\log C$). Curves 1, 1'; 2,2'; 3,3'; 4, 4'; 5, 5'; 6, 6' and 7, 7'correspond to the TX-100 mole fraction in the mixture equal to 0, 0.2; 0.4, 0,5; 0.6, 0.8 and 1, respectively.

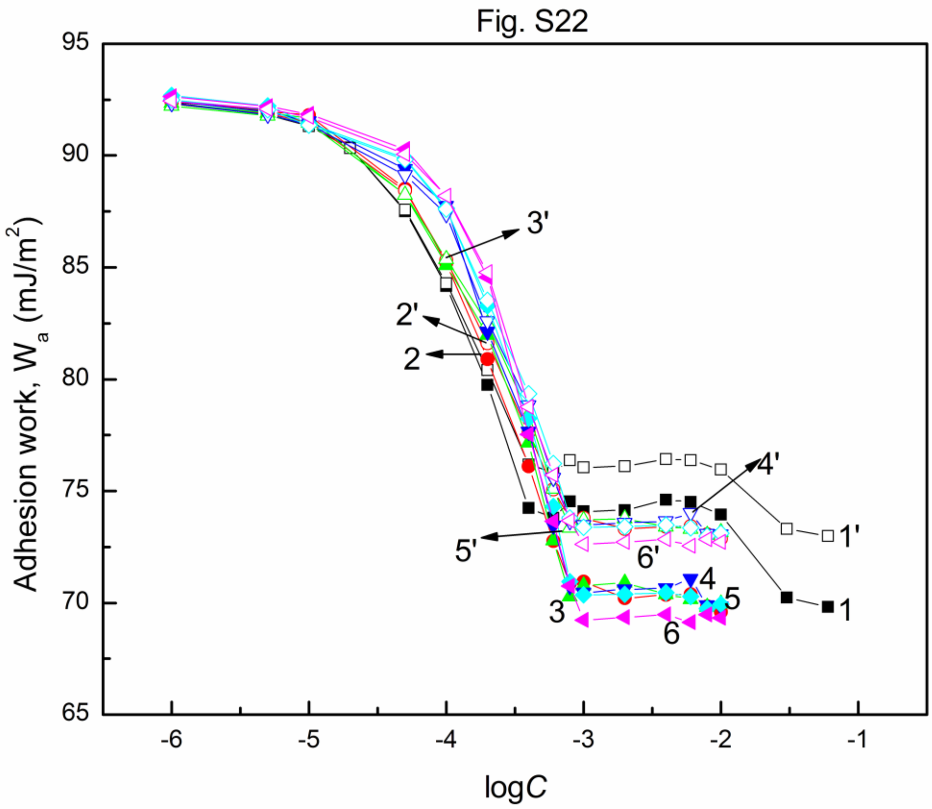

Fig. S22. A plot of the work of adhesion (W_a) of the aqueous solutions of CTAB and CPyB mixtures to the PMMA surface calculated from the Eq. (4) (curves 1 – 7) and Eq. (18) (curves 1' – 7') vs. the logarithm of surfactant mixtures concentration ($\log C$). Curves 1, 1'; 2,2'; 3,3'; 4, 4'; 5, 5' and 6, 6' correspond to the CTAB mole fraction in the mixture equal to 0, 0.2; 0.4, 0.6, 0.8 and 1, respectively.

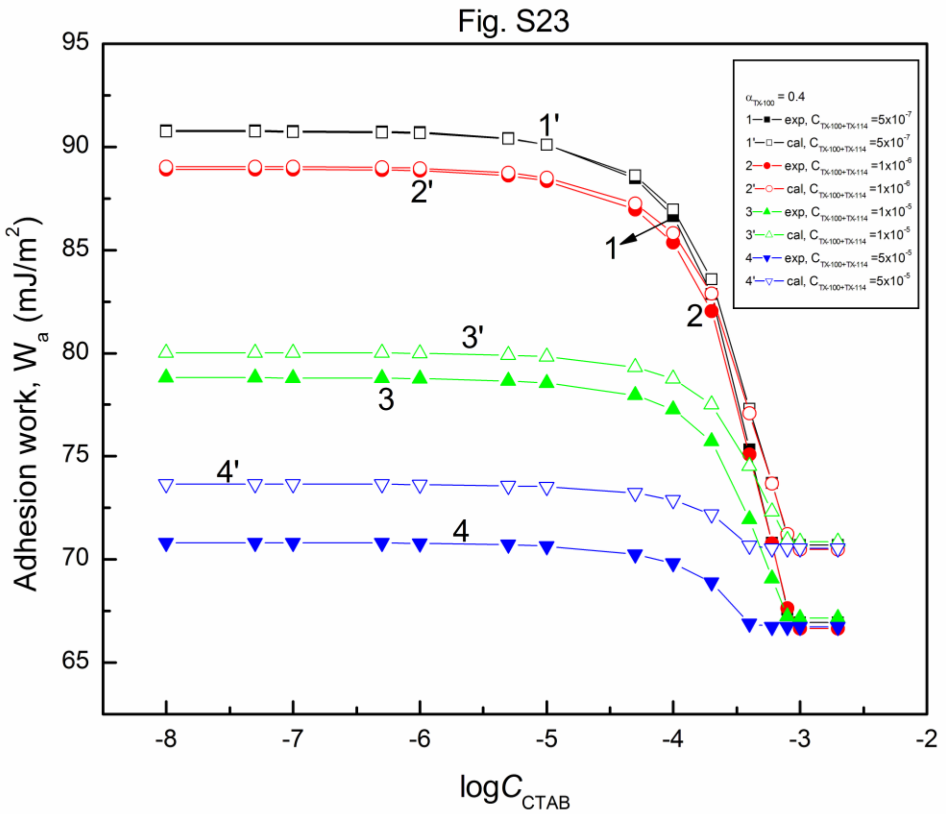

Fig. S23. A plot of the work of adhesion (W_a) of the aqueous solutions of TX-114, TX-100 and CTAB mixtures, at the TX-100 mole fraction in the TX-100+TX-114 mixture α = 0.4, to the PMMA surface calculated from the Eq. (4) (curves 1 – 4) and Eq. (18) (curves 1' – 4') vs. the logarithm of CTAB concentration ($\log C_{CTAB}$). Curves 1, 1'; 2,2'; 3,3' and 4, 4' correspond to the concentration of TX-100+TX-114 mixtures equal to 5 x 10^{-7}, 1 x 10^{-6}, 1 x 10^{-5} and 5 x 10^{-5} M, respectively.

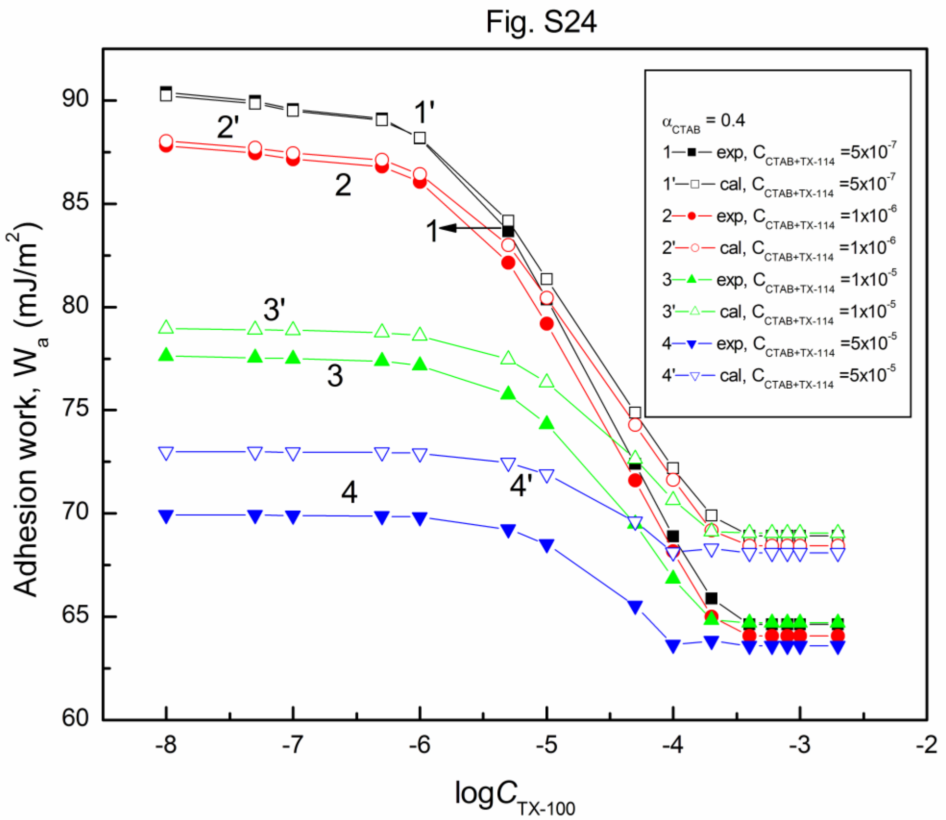

Fig. S24. A plot of the work of adhesion (W_a) of the aqueous solutions of TX-114, TX-100 and CTAB mixtures, at the CTAB mole fraction in the CTAB+TX-114 mixture α = 0.4, to the PMMA surface calculated from the Eq. (4) (curves 1 – 4) and Eq. (18) (curves 1' – 4') vs. the logarithm of TX-100 concentration ($\log C_{TX-100}$). Curves 1, 1'; 2,2'; 3,3' and 4, 4' correspond to the concentration of CTAB+TX-114 mixtures equal to 5 x 10^{-7}, 1 x 10^{-6}, 1 x 10^{-5} and 5 x 10^{-5} M, respectively.

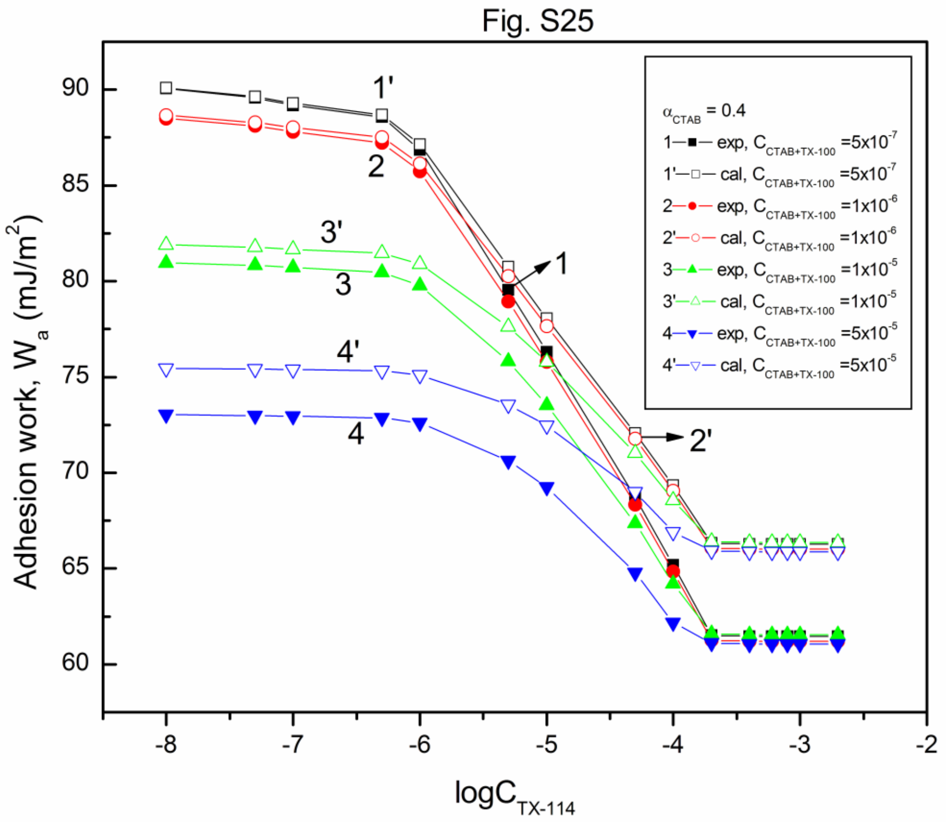

Fig. S25. A plot of the work of adhesion (W_a) of the aqueous solutions of TX-114, TX-100 and CTAB mixtures, at the CTAB mole fraction in the CTAB+TX-100 mixture α = 0.4, to the PMMA surface calculated from the Eq. (4) (curves 1 – 4) and Eq. (18) (curves 1' – 4') vs. the logarithm of TX-114 concentration ($\log C_{TX-114}$). Curves 1, 1'; 2,2'; 3,3' and 4, 4' correspond to the concentration of CTAB+TX-100 mixtures equal to 5 x 10^{-7}, 1 x 10^{-6}, 1 x 10^{-5} and 5 x 10^{-5} M, respectively.

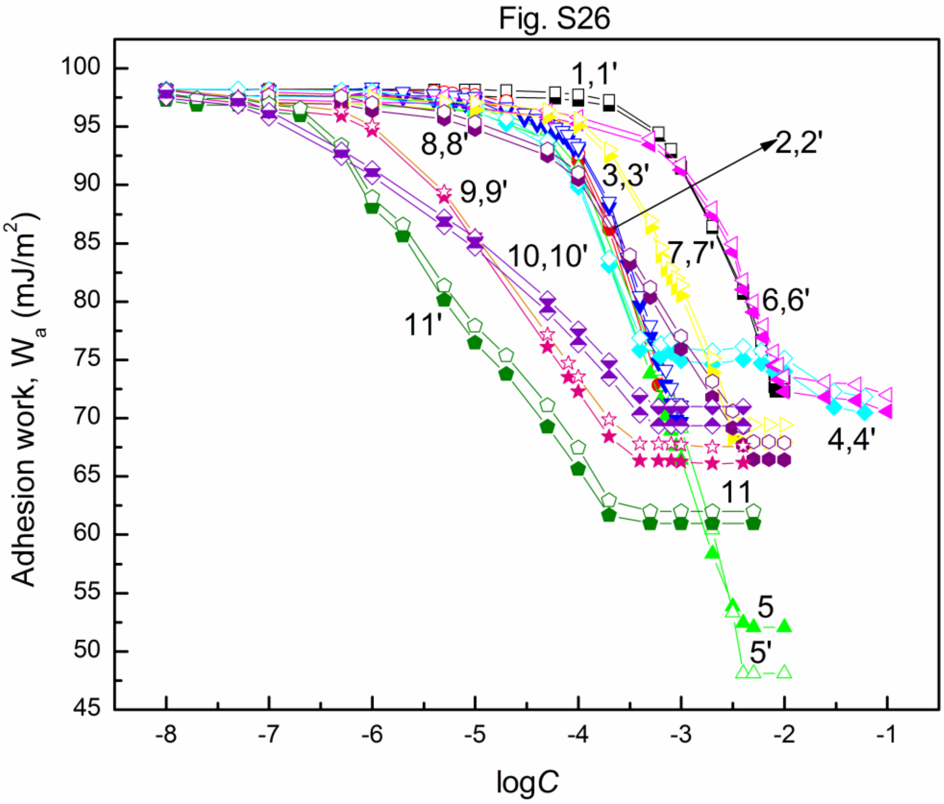

Fig. S26. A plot of the work of adhesion (W_a) of aqueous solutions of surfactants to the nylon 6 surface calculated from the Eq. (4) (curves 1 – 11) and Eq. (18) (curves 1' – 11') vs. the logarithm of surfactant concentration ($\log C$). Curves 1, 1'; 2,2'; 3,3'; 4, 4'; 5, 5'; 6, 6'; 7, 7', 8, 8'; 9, 9'; 10, 10' and 11, 11' correspond to the aqueous solution of SDDS, SHS, SDSa, CTAB, CPyB, DDEAB, TTAB, BDDAB, TX-100, TX-114 and TX-165, respectively.

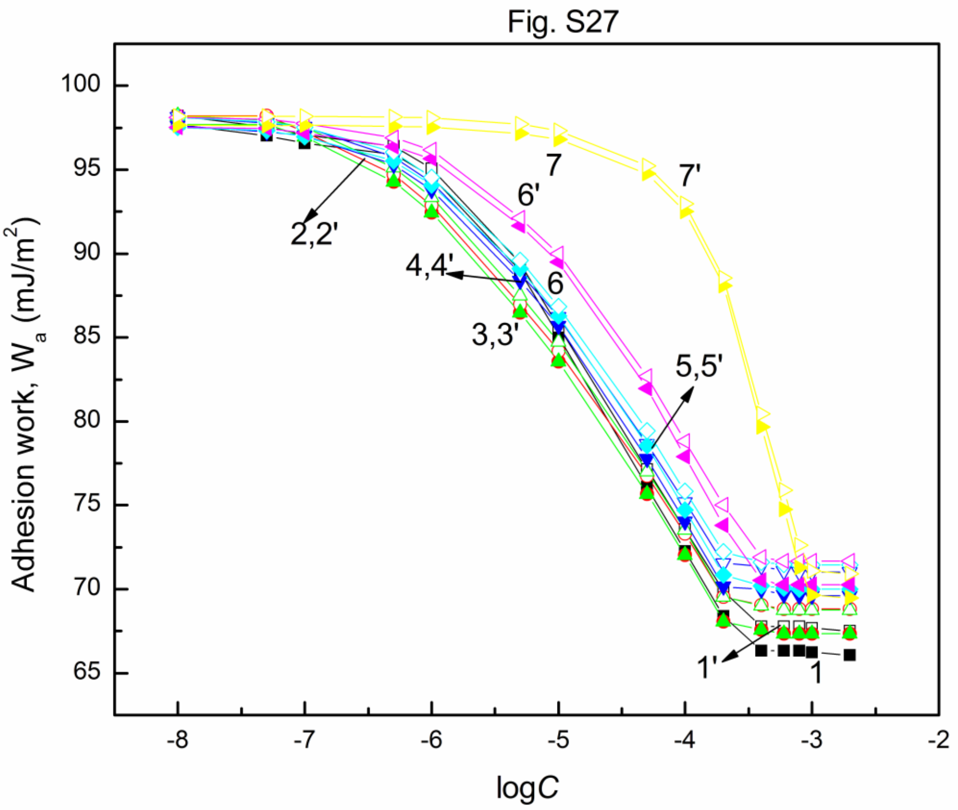

Fig. S27. A plot of the work of adhesion (W_a) of the aqueous solutions of CTAB and TX-100 mixtures to the nylon 6 surface calculated from the Eq. (4) (curves 1 – 7) and Eq. (18) (curves 1' – 7') vs. the logarithm of surfactant mixtures concentration ($\log C$). Curves 1, 1'; 2,2'; 3,3'; 4, 4'; 5, 5'; 6, 6' and 7, 7'correspond to the CTAB mole fractions in the mixture equal to 0, 0.2; 0.4, 0,5; 0.6, 0.8 and 1, respectively.

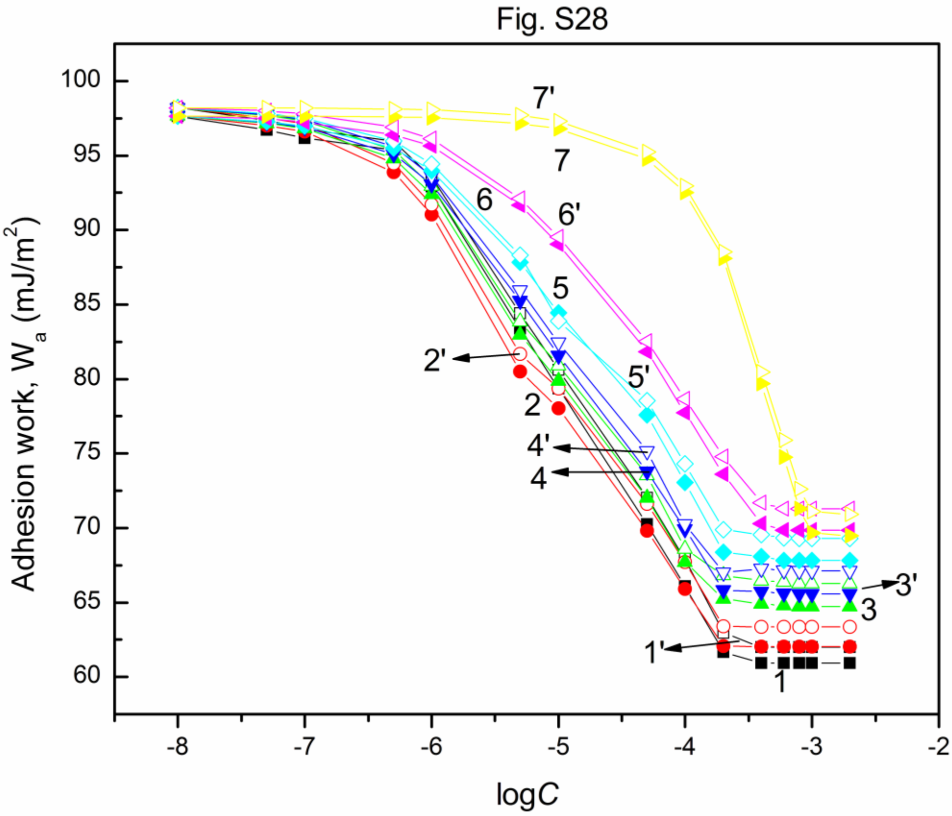

Fig. S28. A plot of the work of adhesion (W_a) of the aqueous solutions of CTAB and TX-114 mixtures to the nylon 6 surface calculated from the Eq. (4) (curves 1 – 7) and Eq. (18) (curves 1' – 7') vs. the logarithm of surfactant mixtures concentration ($\log C$). Curves 1, 1'; 2,2'; 3,3'; 4, 4'; 5, 5'; 6, 6' and 7, 7'correspond to the CTAB mole fractions in the mixture equal to 0, 0.2; 0.4, 0,5; 0.6, 0.8 and 1, respectively.

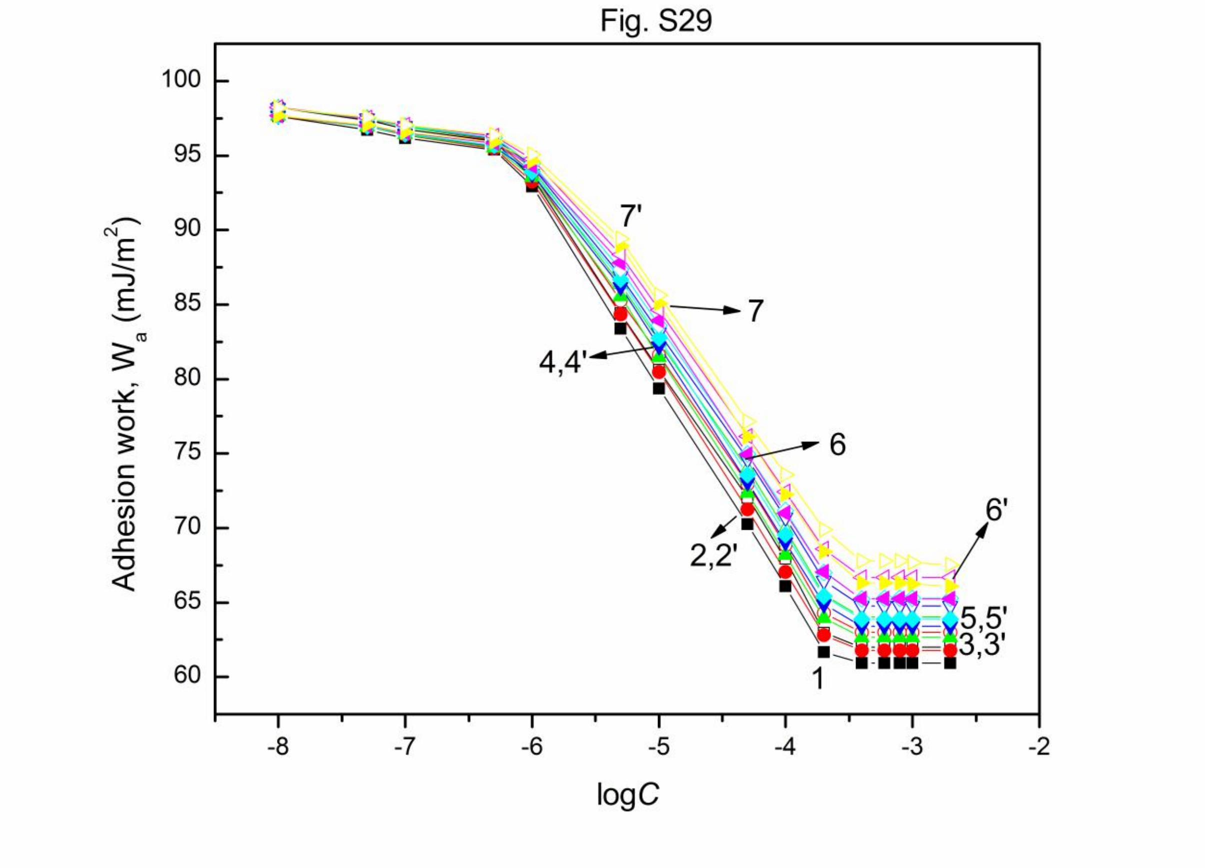

Fig. S29. A plot of the work of adhesion (W_a) of the aqueous solutions of TX-114 and TX-100 mixtures to the nylon 6 surface calculated from the Eq. (4) (curves 1 – 7) and Eq. (18) (curves 1' – 7') vs. the logarithm of surfactant mixtures concentration ($\log C$). Curves 1, 1'; 2,2'; 3,3'; 4, 4'; 5, 5'; 6, 6' and 7, 7'correspond to the TX-100 mole fraction in the mixture equal to 0, 0.2; 0.4, 0,5; 0.6, 0.8 and 1, respectively.

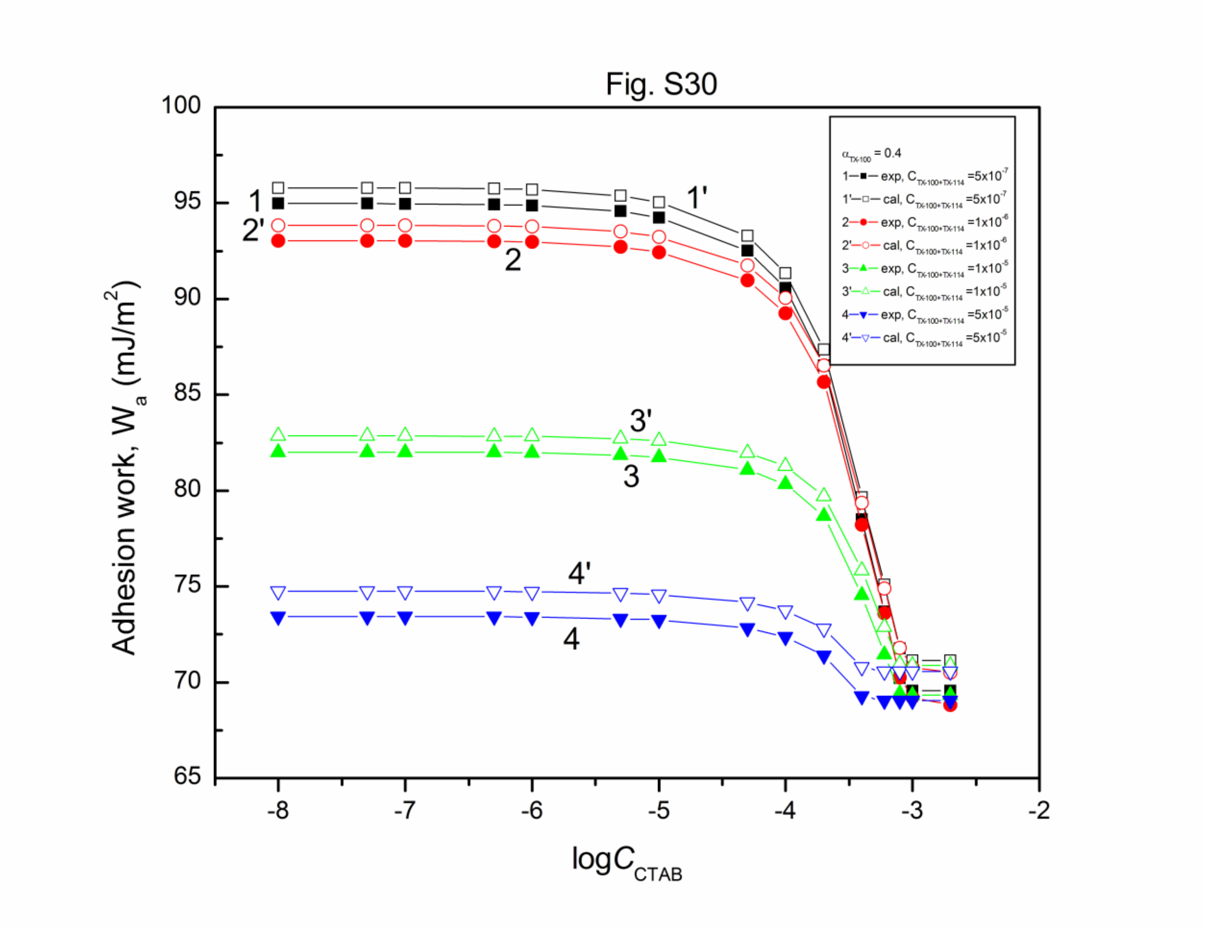

Fig. S30. A plot of the work of adhesion (W_a) of the aqueous solutions of TX-114, TX-100 and CTAB mixtures, at the TX-100 mole fraction in the TX-100+TX-114 mixture α = 0.4, to the nylon 6 surface calculated from the Eq. (4) (curves 1 – 4) and Eq. (18) (curves 1' – 4') vs. the logarithm of CTAB concentration ($\log C_{CTAB}$). Curves 1, 1'; 2,2'; 3,3' and 4, 4' correspond to the concentration of TX-100+TX-114 mixtures equal to 5 x 10^{-7}, 1 x 10^{-6}, 1 x 10^{-5} and 5 x 10^{-5} M, respectively.

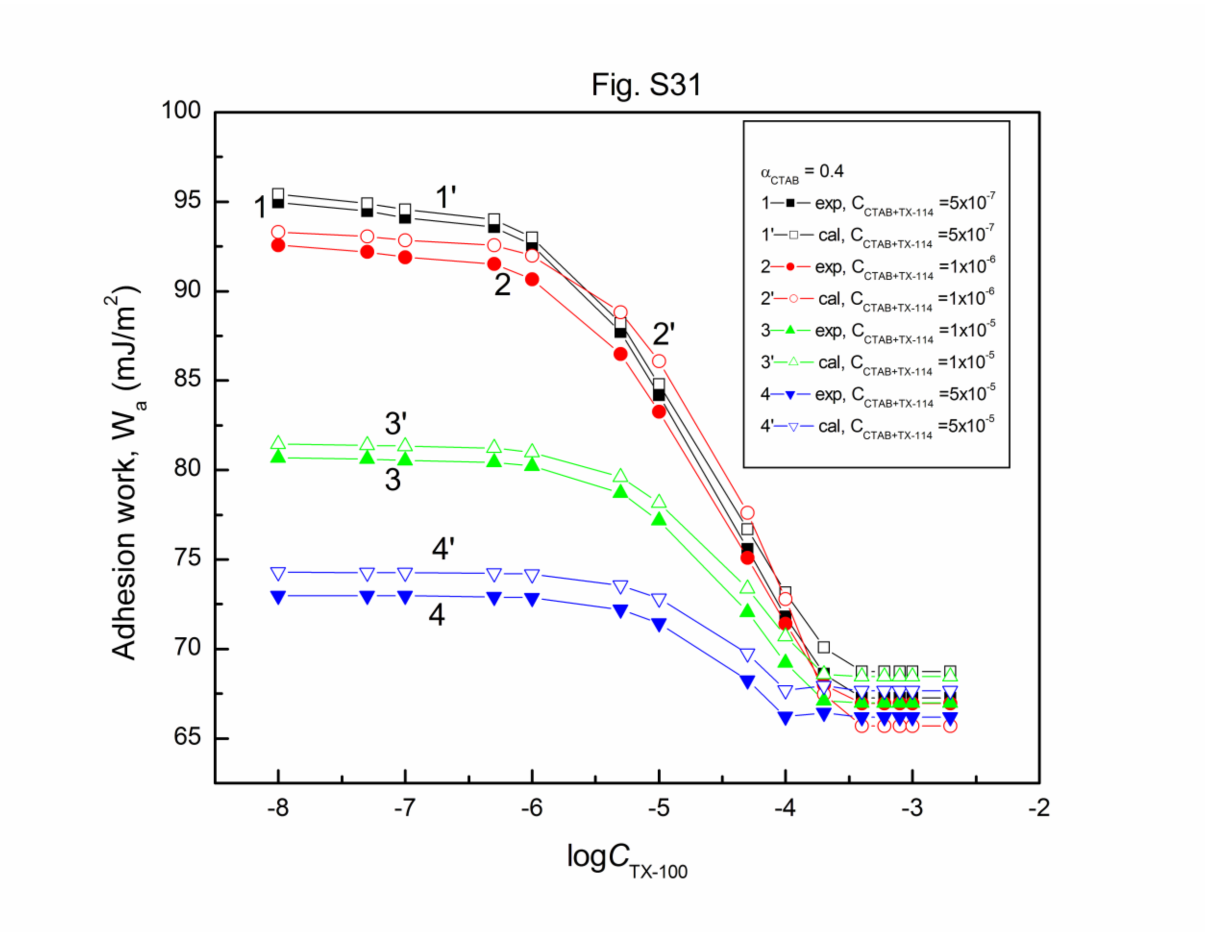

Fig. S31. A plot of the work of adhesion (W_a) of the aqueous solutions of TX-114, TX-100 and CTAB mixtures, at the CTAB mole fraction in the CTAB+TX-114 mixture α = 0.4, to the nylon 6 surface calculated from the Eq. (4) (curves 1 – 4) and Eq. (18) (curves 1' – 4') vs. the logarithm of TX-100 concentration ($\log C_{TX-100}$). Curves 1, 1'; 2,2'; 3,3' and 4, 4' correspond to the concentration of CTAB+TX-114 mixtures equal to 5 x 10^{-7}, 1 x 10^{-6}, 1 x 10^{-5} and 5 x 10^{-5} M, respectively.

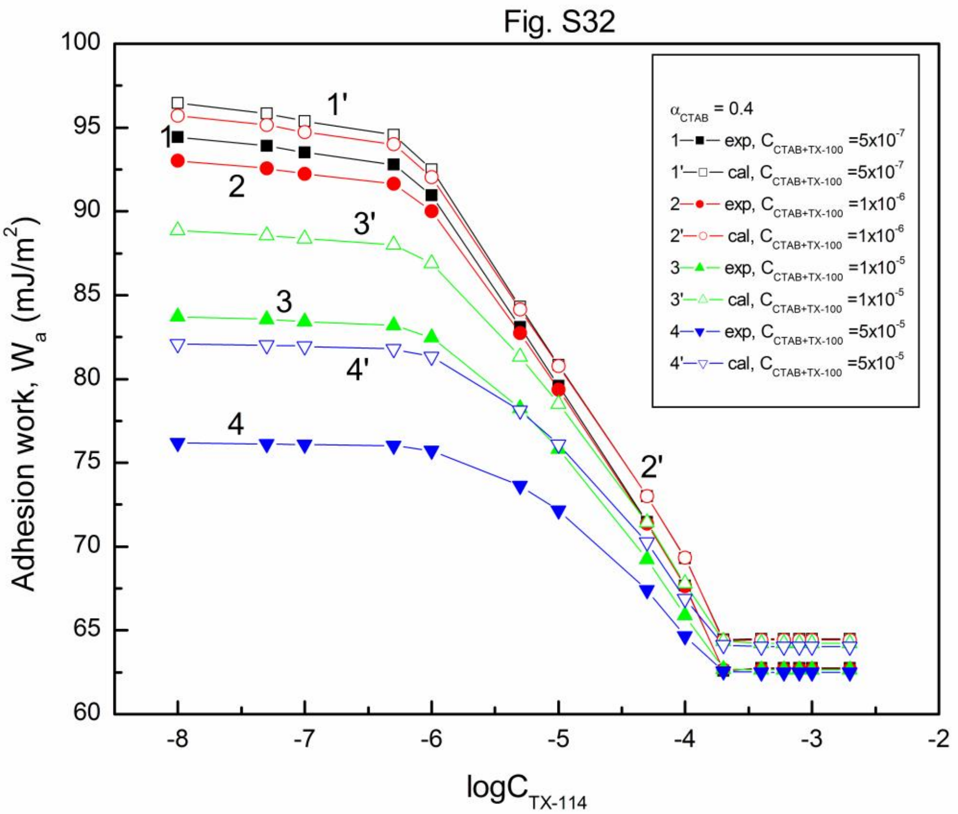

Fig. S32. A plot of the work of adhesion (W_a) of the aqueous solutions of TX-114, TX-100 and CTAB mixtures, at the CTAB mole fraction in the CTAB+TX-100 mixture α = 0.4, to the nylon 6 surface calculated from the Eq. (4) (curves 1 – 4) and Eq. (18) (curves 1’ – 4’) vs. the logarithm of TX-114 concentration ($\log C_{TX-114}$). Curves 1, 1’; 2,2’; 3,3’ and 4, 4’ correspond to the concentration of CTAB+TX-100 mixtures equal to 5 x 10^{-7}, 1 x 10^{-6}, 1 x 10^{-5} and 5 x 10^{-5} M, respectively.